

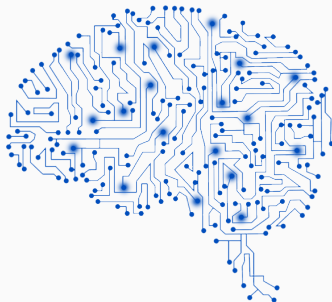
Apprentissage pour l'image

Machine learning for image processing

Course II – Introduction to Artificial Neural Networks: Backpropagation

Emile Pierret

Jeudi 21 mars 2024



At the end of the course :

- Know what is a CNN (Convolutional Neural Network)
- Implement the training of a CNN for classification with Pytorch

For this session :

- Backpropagation to compute gradients in Neural Networks

A simple example

Let consider $f : (x, y) \in \mathbb{R}^2 \mapsto \log(xy)$. How to differentiate f step by step with respect to x ?

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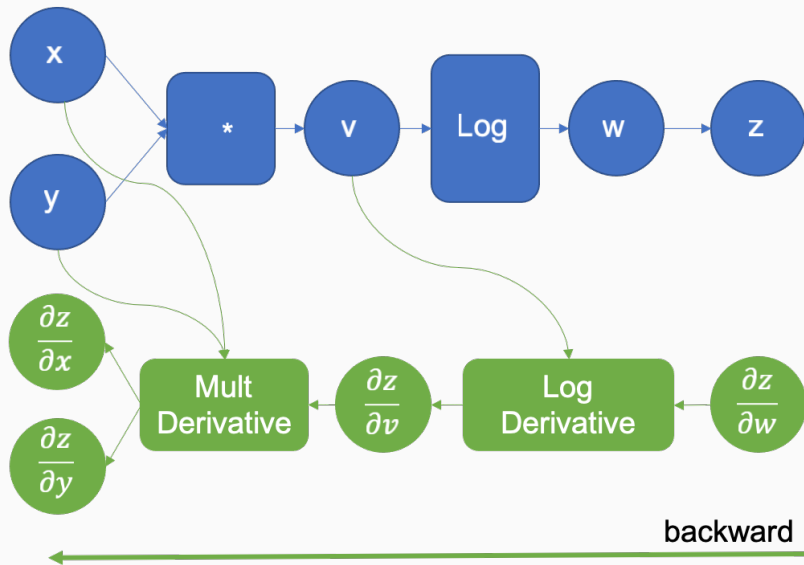
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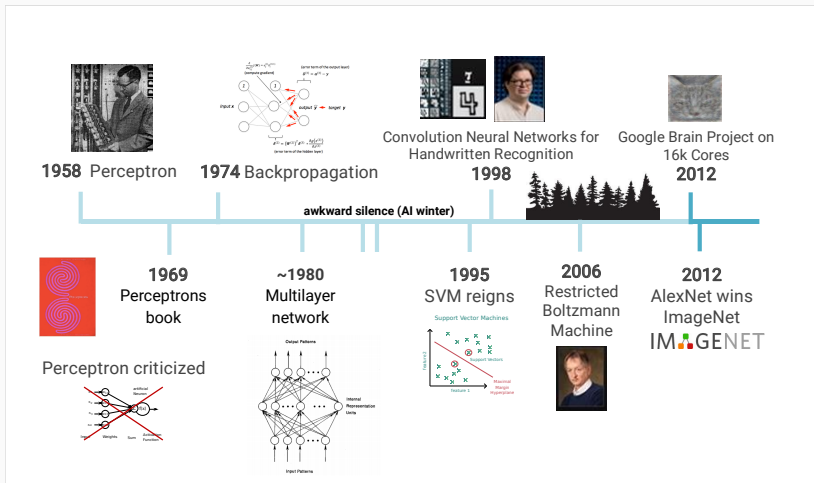
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forward

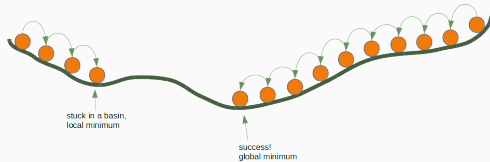


backward

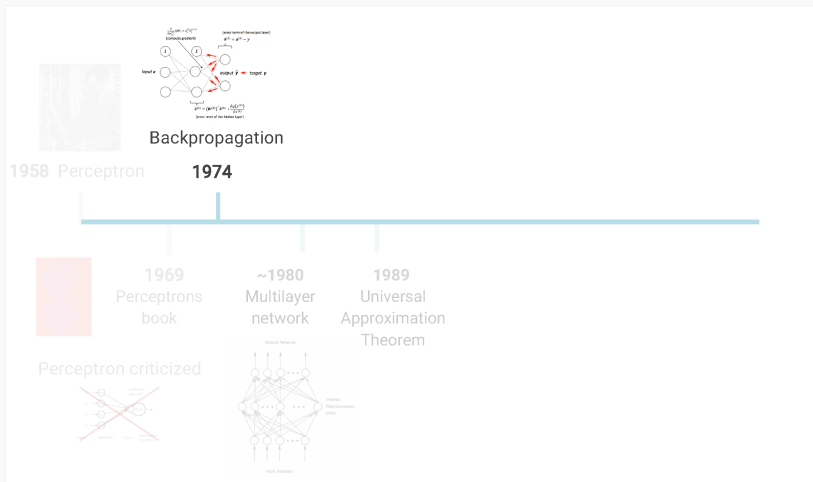
Timeline of (deep) learning



Backpropagation

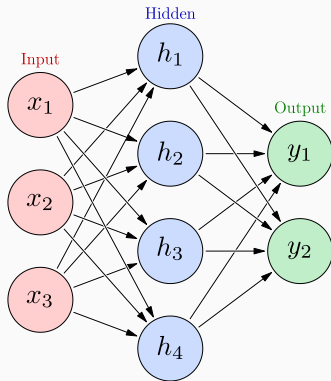


Learning with backpropagation



Feedforward Artificial Neural Network

Artificial neural network / Multilayer perceptron / NeuralNet



$$h_1 = g_1 (w_{11}^1 x_1 + w_{12}^1 x_2 + w_{13}^1 x_3 + b_1^1)$$

$$h_2 = g_1 (w_{21}^1 x_1 + w_{22}^1 x_2 + w_{23}^1 x_3 + b_2^1)$$

$$h_3 = g_1 (w_{31}^1 x_1 + w_{32}^1 x_2 + w_{33}^1 x_3 + b_3^1)$$

$$h_4 = g_1 (w_{41}^1 x_1 + w_{42}^1 x_2 + w_{43}^1 x_3 + b_4^1)$$

$$y_1 = g_2 (w_{11}^2 h_1 + w_{12}^2 h_2 + w_{13}^2 h_3 + w_{14}^2 h_4 + b_1^2)$$

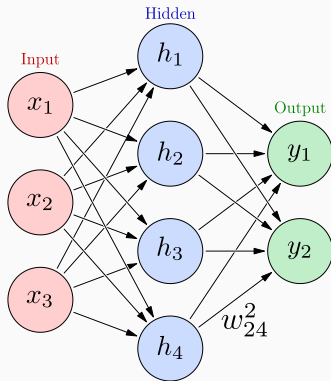
$$y_2 = g_2 (w_{21}^2 h_1 + w_{22}^2 h_2 + w_{23}^2 h_3 + w_{24}^2 h_4 + b_2^2)$$

w_{ij}^k synaptic weight between previous node j and next node i at layer k .

g_k are any activation function applied to each coefficient of its input vector.

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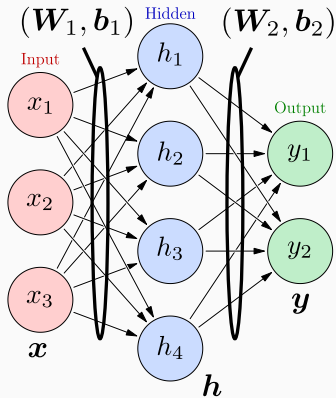
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$$h = g_1 (W_1 x + b_1)$$

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$$y = g_2 (W_2 h + b_2)$$

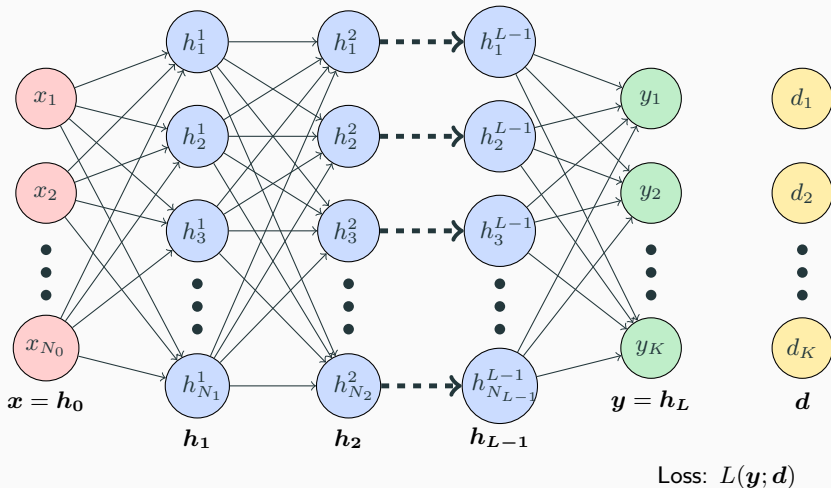
w_{ij}^k synaptic weight between previous node j and next node i at layer k .

g_k are any activation function applied to each coefficient of its input vector.

The matrices W_k and biases b_k are learned from labeled training data.

Feedforward Artificial Neural Network

Recall the feedforward structure



Input Layer

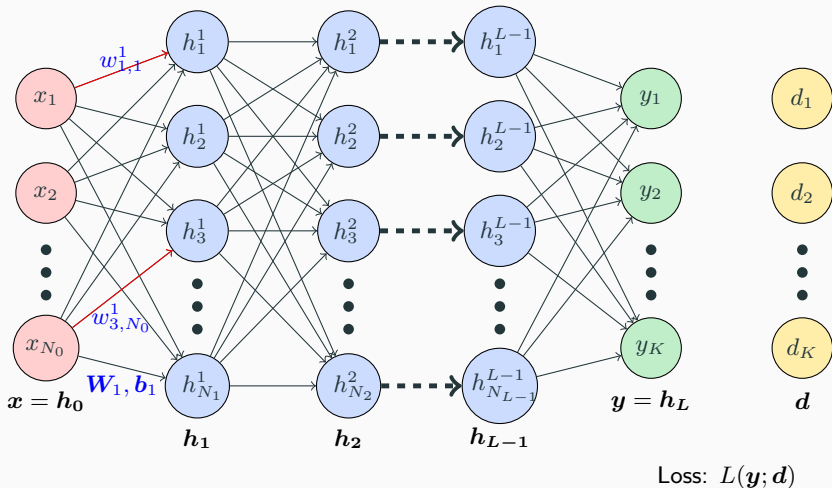
Hidden Layers

Output Layer

Label 8

Feedforward Artificial Neural Network

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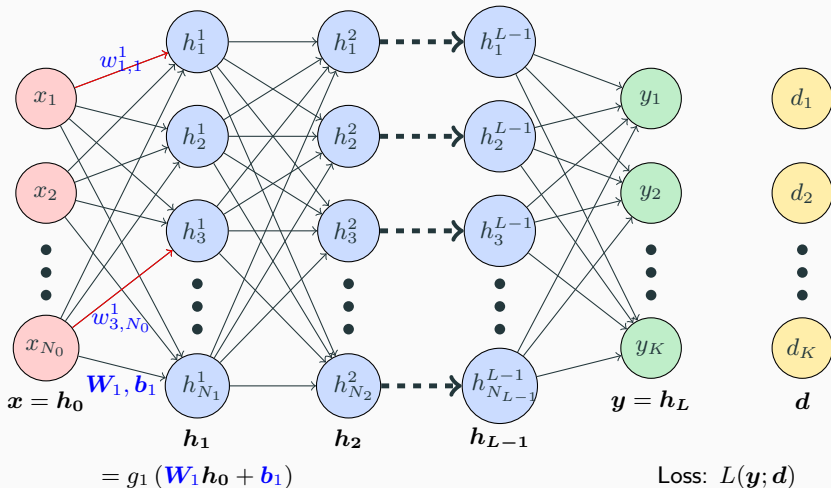
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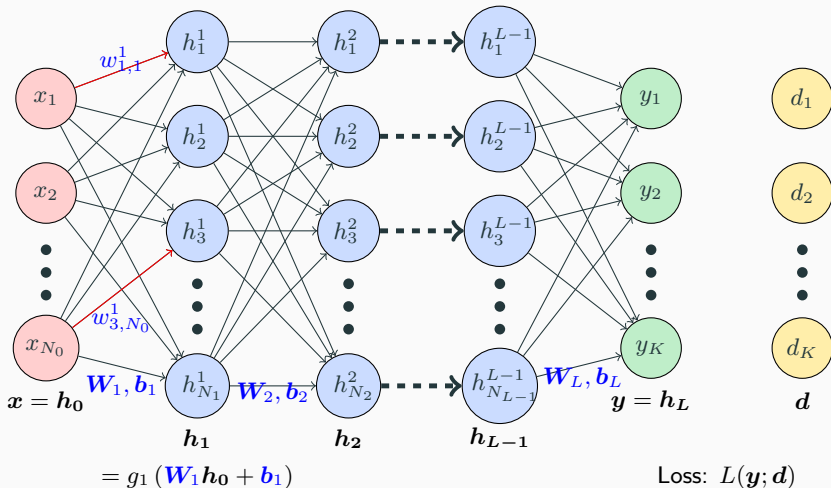
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Feedforward Artificial Neural Network

Recall the feedforward structure



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- The parameters of the neural network are

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Objective: $\min_{\mathbf{W}} E(\mathbf{W})$ where $E(\mathbf{W}) = \sum_{(\mathbf{x}^i, \mathbf{d}^i) \in \mathcal{T}} L(\mathbf{y}^i; \mathbf{d}^i)$

$$\Rightarrow \nabla E(\mathbf{W}) = \left(\frac{\partial E(\mathbf{W})}{\partial \mathbf{W}_1} \quad \frac{\partial E(\mathbf{W})}{\partial \mathbf{b}_1} \quad \dots \quad \frac{\partial E(\mathbf{W})}{\partial \mathbf{W}_L} \quad \frac{\partial E(\mathbf{W})}{\partial \mathbf{b}_L} \right)^T = 0$$

- **Solution:** no closed-form solutions

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- **Solution:** no closed-form solutions \Rightarrow use (stochastic) gradient descent.
- $\frac{\partial E(\mathbf{W})}{\partial \mathbf{W}_k}$ not really rigorous, we will use the notation

$$\nabla_{\mathbf{W}_k} E(\mathbf{W}) \quad \text{and} \quad \nabla_{\mathbf{b}_k} E(\mathbf{W}).$$

Minimizing training loss

For multilayer neural networks $\mathbf{W} \mapsto E(\mathbf{W})$ is non-convex

⇒ No guarantee of convergence.

Even if convergence occurs, the solution depends on the initialization and the step size/learning rate γ .

Nevertheless, really good minima or saddle points are reached in practice by

$$\mathbf{W}^{t+1} \leftarrow \mathbf{W}^t - \gamma \nabla E(\mathbf{W}^t), \quad \gamma > 0$$

Gradient descent can be expressed coordinate by coordinate as:

$$w_{i,j}^{k,t+1} \leftarrow w_{i,j}^{k,t} - \gamma \frac{\partial E(\mathbf{W}^t)}{\partial w_{i,j}^k}$$

for all weights $w_{i,j}^k$ linking a node j to a node i in the next layer k .

⇒ The algorithm to compute $\frac{\partial E(\mathbf{W})}{\partial w_{i,j}^k}$ for ANNs is called **backpropagation**.

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For regression: $\mathbf{d}^i \in \mathbb{R}^K$

- Square error

$$E(\mathbf{W}) = \sum_{(\mathbf{x}^i, \mathbf{d}^i) \in \mathcal{T}} \frac{1}{2} \|\mathbf{y}^i - \mathbf{d}^i\|_2^2 = \sum_{(\mathbf{x}^i, \mathbf{d}^i) \in \mathcal{T}} \frac{1}{2} \sum_k (y_k^i - d_k^i)^2$$

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For multi-class classification: $d^i \in \{1, \dots, K\}$, coded by $\mathbf{d}^i \in \{0, 1\}^K$,

- Cross-entropy with softmax as the last layer

$$E(\mathbf{W}) = - \sum_{(\mathbf{x}^i, \mathbf{d}^i)} \sum_{k=1}^K d_k^i \log y_k^i \quad \text{with} \quad \mathbf{y}^i = f(\mathbf{x}^i; \mathbf{W}) = \text{softmax}(\mathbf{a}^i) \in (0, 1)^K.$$

- Cross-entropy with softmax included in loss (PyTorch convention):

$\mathbf{y}^i = \mathbf{a}^i$ is the output of the last linear layer:

$$E(\mathbf{W}) = - \sum_{(\mathbf{x}^i, \mathbf{d}^i)} \left[a_{d^i} - \log \left(\sum_{k=1}^K \exp(a_k) \right) \right] \quad \text{with } d^i \text{ the class of } \mathbf{x}^i.$$

- The loss functions are of the form

$$E(\mathbf{W}) = \sum_{(\mathbf{x}^i, \mathbf{d}^i)} L(\mathbf{y}^i; \mathbf{d}^i)$$

- By linearity,

$$\nabla E(\mathbf{W}) = \sum_{(\mathbf{x}^i, \mathbf{d}^i)} \nabla L(\mathbf{y}^i; \mathbf{d}^i)$$

- There the neural net output $\mathbf{y}^i = f(\mathbf{x}^i; \mathbf{W})$ is a function of the input data \mathbf{x}^i and the neural weights \mathbf{W} .
- We know the gradient of $L(\mathbf{y}^i; \mathbf{d}^i)$ with respect to the variable \mathbf{y}
 - Regression/Square error:

$$L(\mathbf{y}; \mathbf{d}) = \frac{1}{2} \|\mathbf{y} - \mathbf{d}\|_2^2 \quad \Rightarrow \quad \nabla_{\mathbf{y}} L(\mathbf{y}; \mathbf{d}) = \mathbf{y} - \mathbf{d}$$

- Multi-class classification/cross-entropy:

$$L(\mathbf{y}; \mathbf{d}) = -y_d + \log \left(\sum_{k=1}^K \exp(y_k) \right) \Rightarrow (\nabla_{\mathbf{y}} L(\mathbf{y}; \mathbf{d}))_{\ell} = \text{softmax}(\mathbf{y})_{\ell} - \delta_{\ell, d}.$$

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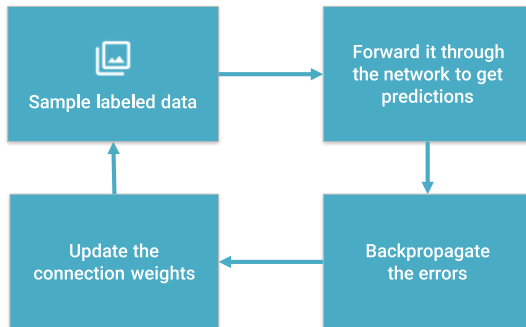
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- We know the gradient of $L(\mathbf{y}^i; \mathbf{d}^i)$ with respect to the variable \mathbf{y}
- We still need to compute

$$\nabla_{\mathbf{W}_k} L(\mathbf{y}; \mathbf{d}) \quad \text{and} \quad \nabla_{\mathbf{b}_k} L(\mathbf{y}; \mathbf{d}) \quad \text{for } k = 0, \dots, L.$$

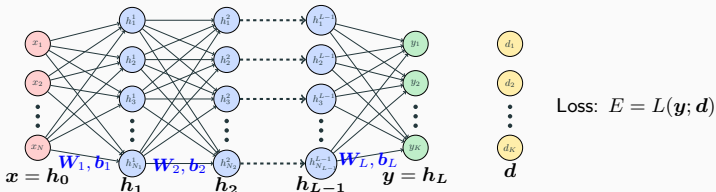
- For simplicity above we will use the notation $E = L(\mathbf{y}; \mathbf{d})$, that is considering only one point.

Training process



Learns by generating an error signal that measures the difference between the predictions of the network and the desired values and then **using this error signal to change the weights** (or parameters) so that predictions get more accurate.

ANN – Backpropagation



Forward pass

Initialization:

$$h_0 = x$$

for layer $k = 1$ **to** L **do**

Linear unit:

$$a_k = W_k h_{k-1} + b_k$$

Componentwise non-linear activation:

$$h_k = g_k(a_k)$$

end

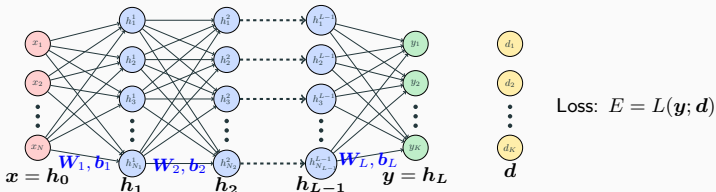
Output layer:

$$y = h_L$$

Compute loss:

$$E = L(y; d)$$

ANN – Backpropagation



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for layer $k = 1$ **to** L **do**

Linear unit:

$$\mathbf{a}_k = \mathbf{W}_k \mathbf{h}_{k-1} + \mathbf{b}_k$$

Componentwise non-linear activation:

$$\mathbf{h}_k = g_k(\mathbf{a}_k)$$

end

Output layer:

$$\mathbf{y} = \mathbf{h}_L$$

Compute loss:

$$E = L(\mathbf{y}; \mathbf{d})$$

Backward pass

Goal: Compute the gradient with respect to all parameters

$$\frac{\partial E}{\partial w_{i,j}^k} = ? \quad \frac{\partial E}{\partial b_i^k} = ?$$

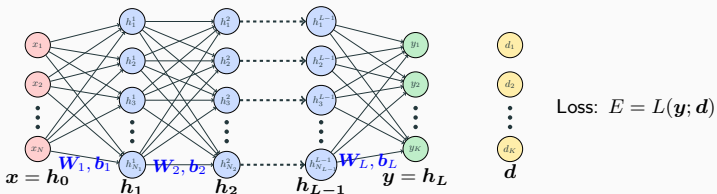
for all

$$k \in \{1, \dots, L\},$$

$$i \in \{1, \dots, N_k\},$$

$$j \in \{1, \dots, N_{k-1}\}.$$

ANN – Backpropagation

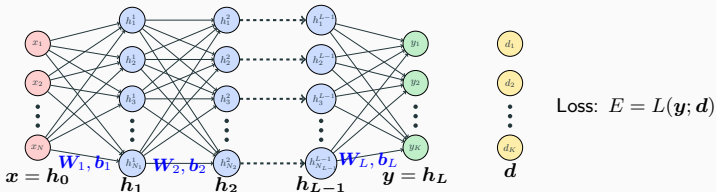


Going backward

- We know how to compute the loss function and its gradient:

$$\nabla_{h_L} E = \nabla L(y; d)$$

ANN – Backpropagation



Gradient with respect to last linear unit output a_L

$$h_L = g_L(a_L)$$

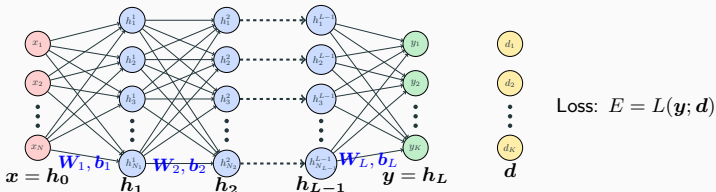
That is for all $i \in \{1, \dots, N_L\}$, $h_i^L = g_L(a_i^L)$. By the chain rule,

$$\frac{\partial E}{\partial a_i^L} = \frac{\partial E}{\partial h_i^L} \frac{\partial h_i^L}{\partial a_i^L} = [\nabla_{h_L} E]_i g'_L(a_i^L)$$

Vector formula: $\nabla_{a_L} E = \nabla_{h_L} E \odot g'_L(a_L)$

where \odot is the componentwise product between vectors, ie Hadamard product.

ANN – Backpropagation



Gradient with respect to bias of last linear unit b_L

$$a_L = W_L h_{L-1} + b_L$$

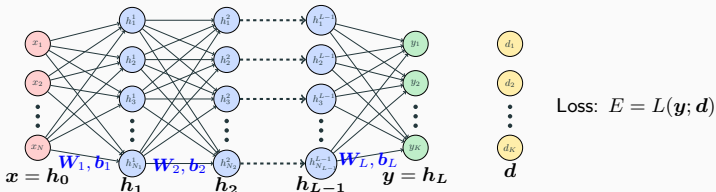
That is for all $i \in \{1, \dots, N_L\}$, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.

By the chain rule, for all $i \in \{1, \dots, N_L\}$,

$$\frac{\partial E}{\partial b_i^L} = \frac{\partial E}{\partial a_i^L} \underbrace{\frac{\partial a_i^L}{\partial b_i^L}}_{=1} = \frac{\partial E}{\partial a_i^L} = [\nabla_{a_L} E]_i$$

Vector formula: $\nabla_{b_L} E = \nabla_{a_L} E$

ANN – Backpropagation



Gradient with respect to weights of last linear unit W_L

$$a_L = W_L h_{L-1} + b_L$$

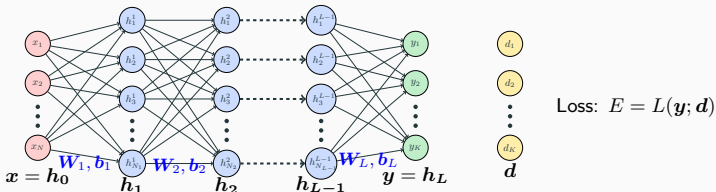
That is for all $i \in \{1, \dots, N_L\}$, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.

By the chain rule, for all $i \in \{1, \dots, N_L\}$ and $j \in \{1, \dots, N_{L-1}\}$

$$\frac{\partial E}{\partial w_{i,j}^L} = \frac{\partial E}{\partial a_i^L} \underbrace{\frac{\partial a_i^L}{\partial w_{i,j}^L}}_{=h_j^{L-1}} = \frac{\partial E}{\partial a_i^L} h_j^{L-1} = [\nabla_{a_L} E]_i [h_{L-1}]_j$$

Matrix formula: $\nabla_{W_L} E = \nabla_{a_L} E h_{L-1}^T$

ANN – Backpropagation

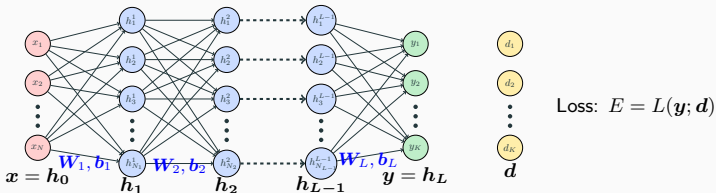


Gradients for last layer parameters

Given the gradient with respect to the output layer $\nabla_{h_L} E$, so far we can compute:

- $\nabla_{\mathbf{a}_L} E = \nabla_{h_L} E \odot g'_L(\mathbf{a}_L)$
- $\nabla_{\mathbf{b}_L} E = \nabla_{\mathbf{a}_L} E$
- $\nabla_{\mathbf{W}_L} E = \nabla_{\mathbf{a}_L} E \mathbf{h}_{L-1}^T$

ANN – Backpropagation



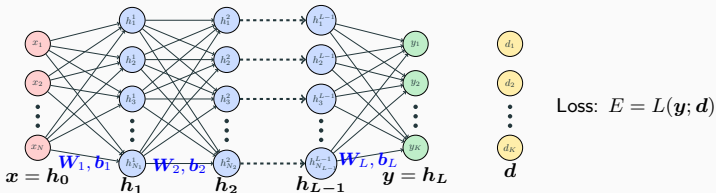
Gradients for last layer parameters

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How can we compute the gradients for the parameters of layer $L - 1$?

ANN – Backpropagation



Gradients for last layer parameters

Given the gradient with respect to the output layer $\nabla_{h_L} E$, so far we can compute:

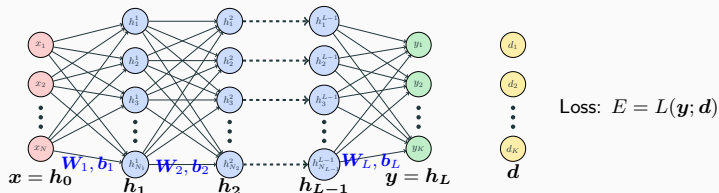
- $\nabla_{a_L} E = \nabla_{h_L} E \odot g'_L(a_L)$
- $\nabla_{b_L} E = \nabla_{a_L} E$
- $\nabla_{W_L} E = \nabla_{a_L} E h_{L-1}^T$

How can we compute the gradients for the parameters of layer $L - 1$?

We need the expression of the gradient with respect to the last but one hidden layer h_{L-1} ... and then the same formulas apply!

$$\nabla_{h_{L-1}} E = ?$$

ANN – Backpropagation

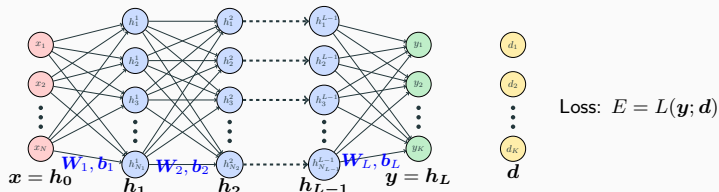


Gradient with respect to the last but one hidden layer h_{L-1}

Here, even to compute the scalar partial derivative $\frac{\partial E}{\partial h_j^{L-1}}$, we need to use differential calculus for multivariate functions since h_j^{L-1} appears in each component of a_L :

$$\text{For all } i \in \{1, \dots, N_L\}, a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L.$$

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Gradient with respect to the last but one hidden layer h_{L-1}

Let us recall the derivative rule for composition with affine maps:

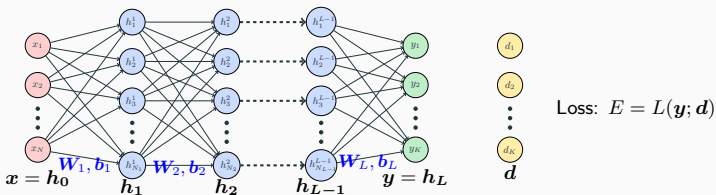
$$\text{For } \varphi(x) = f(Ax + b) \text{ one has } \nabla \varphi(x) = A^T \nabla f(Ax + b).$$

Using the decomposition

$$\begin{aligned} \mathbb{R}^{N_{L-1}} &\rightarrow \mathbb{R}^{N_L} \rightarrow \mathbb{R} \\ h_{L-1} &\mapsto a_L = W_L h_{L-1} + b_L \mapsto E \end{aligned}$$

$$\text{Vector formula: } \nabla_{h_{L-1}} E = W_L^T \nabla_{a_L} E$$

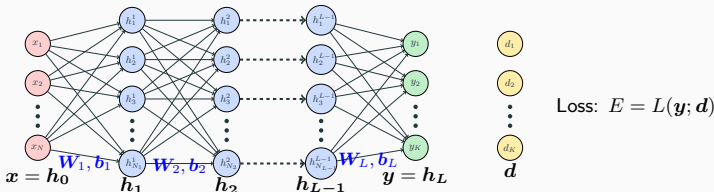
ANN – Backpropagation



We know $\nabla_{h_{L-1}} E$ and :

- $h_{L-1} = g_{L-1}(a_{L-1}) \Rightarrow \nabla_{a_{L-1}} E = \nabla_{h_{L-1}} E \odot g'_{L-1}(a_{L-1})$
- $a_{L-1} = W_{L-1} h_{L-2} + b_{L-1}$
- As before,
- $\nabla_{b_{L-1}} E = \nabla_{a_{L-1}} E$
- $\nabla_{W_{L-1}} E = \nabla_{a_{L-1}} E h_{L-2}^T$

ANN – Backpropagation



Forward pass

Initialization:

$$\mathbf{h}_0 = \mathbf{x}$$

for layer $k = 1$ **to** L **do**

Linear unit:

$$\mathbf{a}_k = \mathbf{W}_k \mathbf{h}_{k-1} + \mathbf{b}_k$$

Componentwise non-linear activation:

$$\mathbf{h}_k = g_k(\mathbf{a}_k)$$

end

Output layer:

$$\mathbf{y} = \mathbf{h}_L$$

Compute loss:

$$E = L(\mathbf{y}; \mathbf{d})$$

Backward pass

Initialization: Gradient of output layer:

$$\nabla_{\mathbf{h}_L} E = \nabla L(\mathbf{y}; \mathbf{d})$$

for layer $k = L$ **to** 1 **do**

Componentwise gain of error:

$$\delta_k = \nabla_{\mathbf{a}_k} E = \nabla_{\mathbf{h}_k} E \odot g'_k(\mathbf{a}_k)$$

Gradient of layer bias:

$$\nabla_{\mathbf{b}_k} E = \delta_k$$

Gradient of weights:

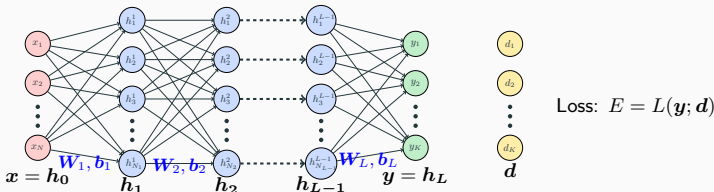
$$\nabla_{\mathbf{W}_k} E = \delta_k \mathbf{h}_{k-1}^T$$

Gradient of previous hidden layer:

$$\nabla_{\mathbf{h}_{k-1}} E = \mathbf{W}_k^T \delta_k$$

end

ANN – Backpropagation



Forward pass

Initialization:

$$\mathbf{h}_0 = \mathbf{x}$$

for layer $k = 1$ **to** L **do**

Linear unit:

$$\mathbf{a}_k = \mathbf{W}_k \mathbf{h}_{k-1} + \mathbf{b}_k \text{ (stored)}$$

Componentwise non-linear activation:

$$\mathbf{h}_k = g_k(\mathbf{a}_k) \text{ (stored)}$$

end

Output layer:

$$\mathbf{y} = \mathbf{h}_L$$

Compute loss:

$$E = L(\mathbf{y}; \mathbf{d})$$

Backward pass

Initialization: Gradient of output layer:

$$\nabla_{\mathbf{h}_L} E = \nabla L(\mathbf{y}; \mathbf{d})$$

for layer $k = L$ **to** 1 **do**

Componentwise gain of error:

$$\delta_k = \nabla_{\mathbf{a}_k} E = \nabla_{\mathbf{h}_k} E \odot g'_k(\mathbf{a}_k)$$

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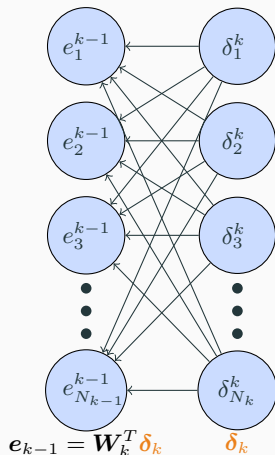
$$\nabla_{\mathbf{W}_k} E = \delta_k \mathbf{h}_{k-1}^T$$

Gradient of previous hidden layer:

$$\nabla_{\mathbf{h}_{k-1}} E = \mathbf{W}_k^T \delta_k$$

end

Error backpropagation

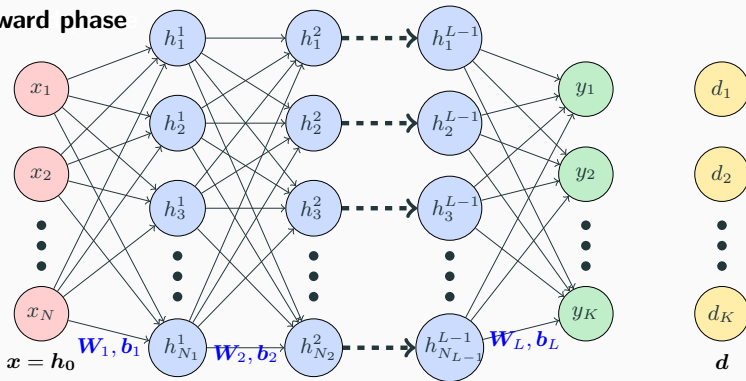


- Gradient of previous hidden layer:

$$e_{k-1} = \nabla_{h_{k-1}} E = \mathbf{W}_k^T \delta_k$$
- Multiplying by \mathbf{W}_k^T corresponds to passing to the linear layer in reverse order.
- The error is backpropagated layer by layer to compute the gradient with respect to each layer parameters.

Error backpropagation

Forward phase



Input Layer

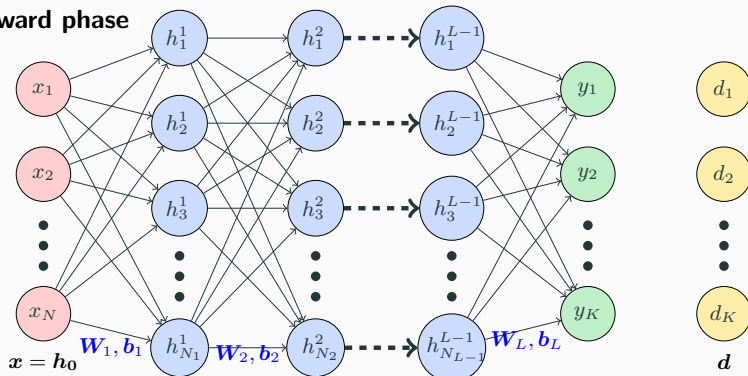
Hidden Layers

Output Layer

Label

Error backpropagation

Forward phase



$$a_1 = W_1 h_0 + b_1$$

$$h_1 = g_1(a_1)$$

$$L = \sum_{k=1}^K (y_k - d_k)^2$$

Input Layer

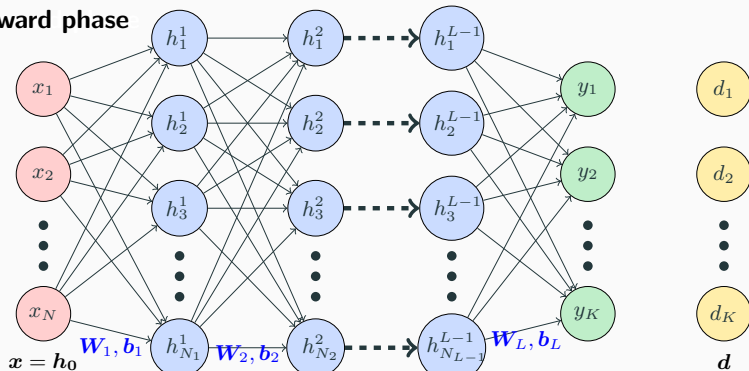
Hidden Layers

Output Layer

Label

Error backpropagation

Forward phase



Input Layer

Hidden Layers

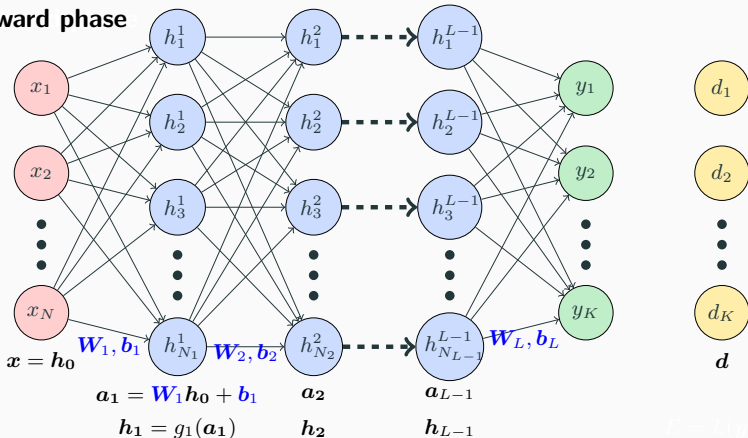
Output Layer

Label

ANN – Backpropagation

Error backpropagation

Forward phase



Input Layer

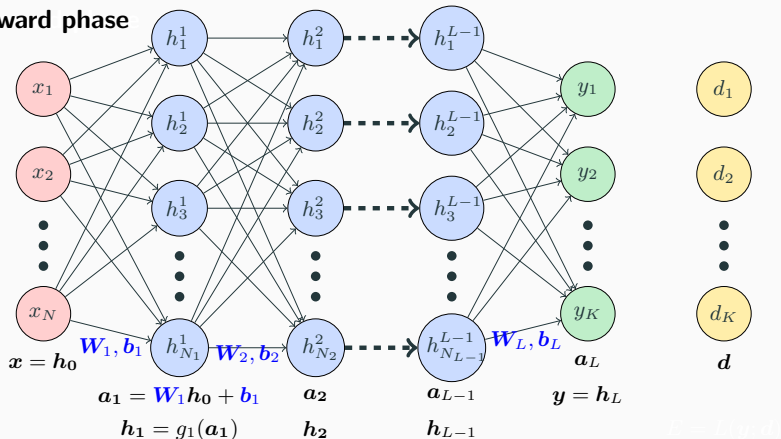
Hidden Layers

Output Layer

Label

Error backpropagation

Forward phase



Input Layer

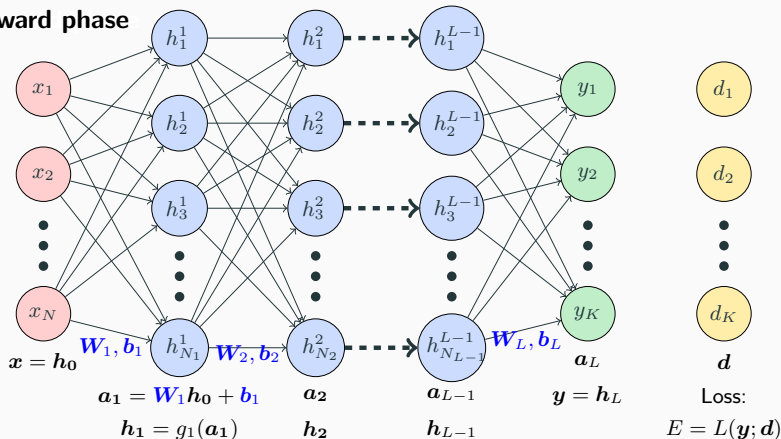
Hidden Layers

Output Layer

Label

Error backpropagation

Forward phase



Input Layer

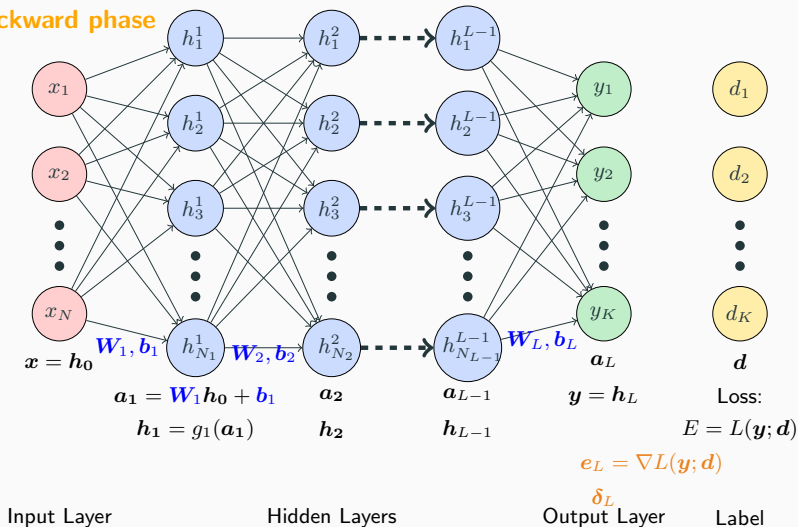
Hidden Layers

Output Layer

Label

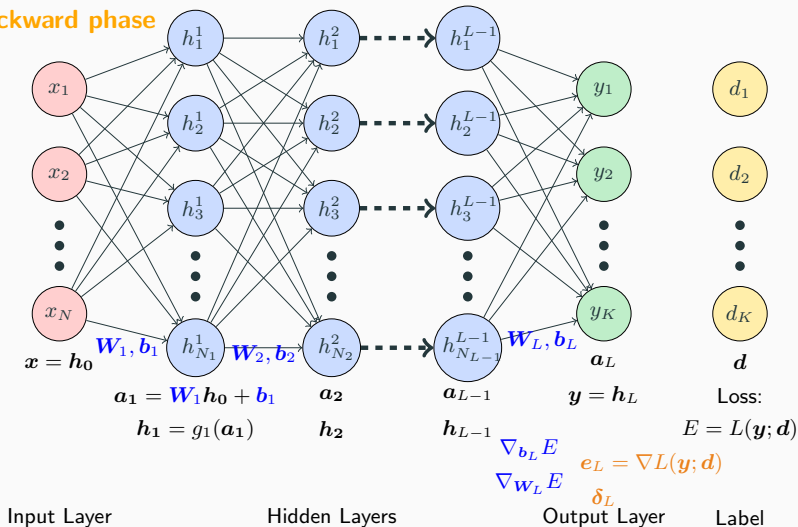
Error backpropagation

Backward phase



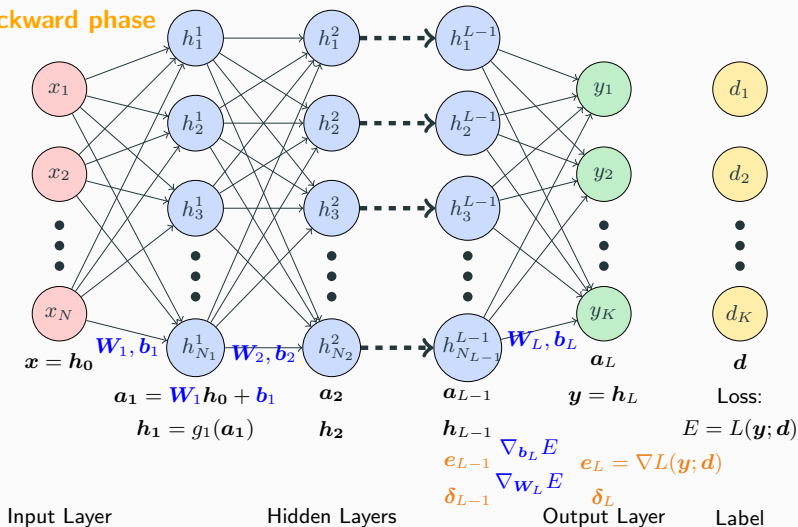
Error backpropagation

Backward phase



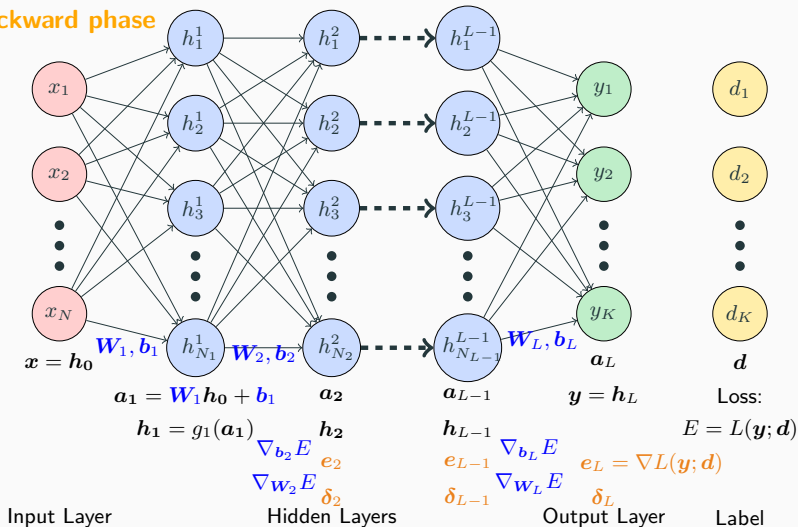
Error backpropagation

Backward phase



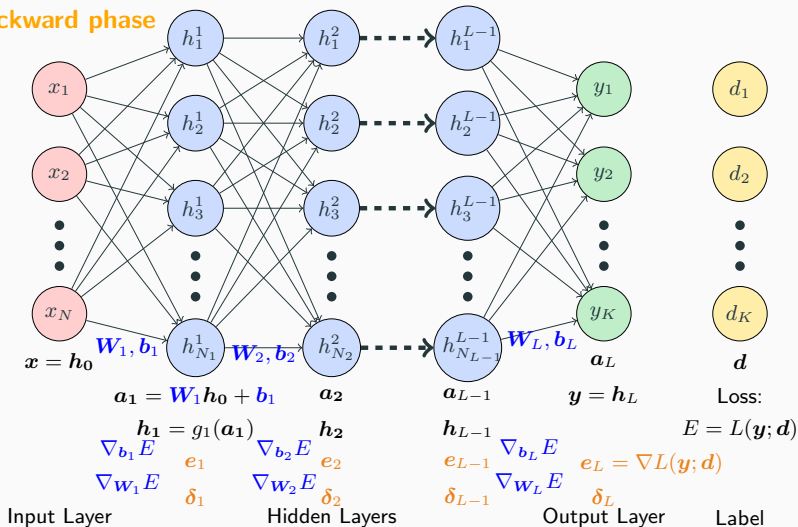
Error backpropagation

Backward phase



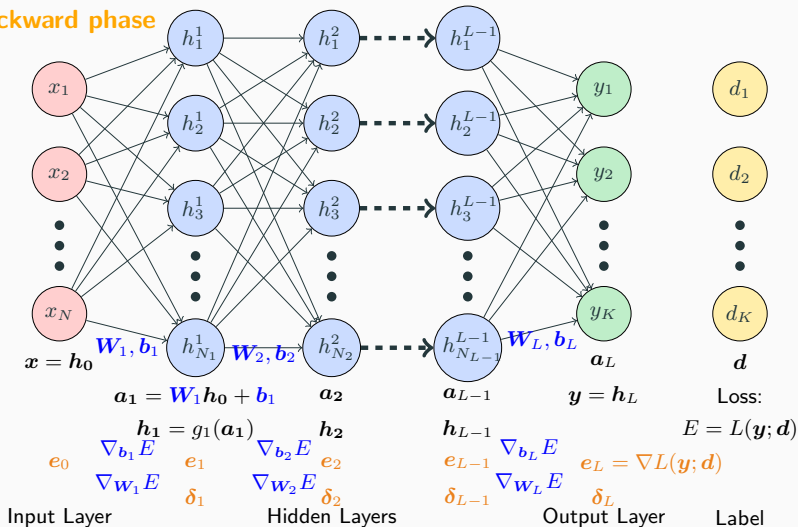
Error backpropagation

Backward phase



Error backpropagation

Backward phase



Error backpropagation in practice

Training loss:

$$E(\mathbf{W}) = \sum_{(\mathbf{x}^i, \mathbf{d}^i) \in \mathcal{T}} L(\mathbf{y}^i; \mathbf{d}^i)$$

- The backpropagation procedure computes $\nabla_{\mathbf{W}} L(\mathbf{y}^i; \mathbf{d}^i) = \nabla_{\mathbf{W}} L(f(\mathbf{x}^i; \mathbf{W}); \mathbf{d}^i)$.
- This has to be done for each data point $\mathbf{x}^i \in \mathcal{T}$.
- By linearity, the final gradient $\nabla E(\mathbf{W})$ is the sum of all individual gradients $\nabla_{\mathbf{W}} L(\mathbf{y}^i; \mathbf{d}^i)$.
- These gradients are summed sequentially (no need to store each individual gradients).
- In general we do not compute the exact gradient...

Error backpropagation in practice

Batch loss:

$$E(\mathbf{W}) \approx \sum_{(\mathbf{x}^i, \mathbf{d}^i) \in \mathcal{S}} L(\mathbf{y}^i; \mathbf{d}^i), \quad \text{with } \mathcal{S} \subset \mathcal{T}$$

- The backpropagation has to be done for each visited data point $\mathbf{x}^i \in \mathcal{S}$ of the batch.
- The gradient for each point \mathbf{x}^i is added to the running gradient = current gradient estimation.
- Once the noisy estimated gradient is used as a gradient step, one needs to set the gradients to zero: See PyTorch `torch.zero_grad()` procedure.

Why is the backpropagation so efficient ?

- Avoid to re-do numerous computations
- No parameters need to be tuned
- Easy to implement
- This method can be seen as a Jacobian multiplication "in the right direction"

Some limitations :

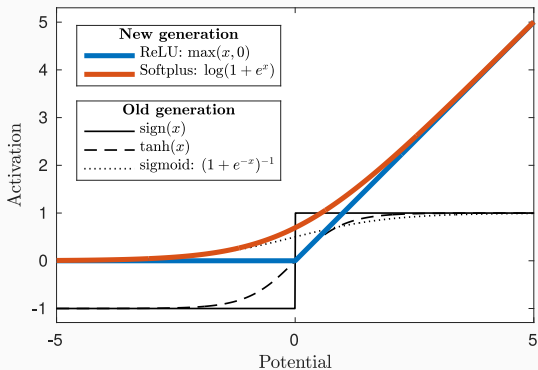
- Memory consuming
- Backpropagation learning does not require normalization of input vectors; however, normalization could improve performance.

Go back on 'on comprendra plus tard'

Considering

$$\mathbf{h}_{L-1} = g_{L-1}(\mathbf{a}_{L-1}) \Rightarrow \nabla_{\mathbf{a}_{L-1}} E = \nabla_{\mathbf{h}_{L-1}} E \odot g'_{L-1}(\mathbf{a}_{L-1})$$

Why ReLU is preferable to sign ?



Stochastic gradient in practice

$$L(\mathbf{W}) = \sum_{\mathbf{x} \in \mathcal{E}} \ell(\mathbf{x}, \mathbf{W})$$

On découpe l'ensemble de données \mathcal{T} en "batches" \mathcal{S} tels que $\mathcal{T} = \bigcup \mathcal{S}$

Comment optimiser le réseau ?

$$L(\mathbf{W}) = \sum_{\mathbf{x} \in \mathcal{E}} \ell(\mathbf{x}, \mathbf{W})$$

On découpe l'ensemble de données \mathcal{T} en "batches" \mathcal{S} tels que $\mathcal{T} = \bigcup \mathcal{S}$

- Pour chaque époque :
 - Pour chaque batch \mathcal{B} de l'ensemble de données d'entraînement, pris dans un ordre aléatoire
 - Calculer $\ell(W, \mathbf{x})$ pour \mathbf{x} dans le batch
 - Calculer $\mathbf{g} = \sum_{\mathbf{x} \in \mathcal{B}} \nabla_{\mathbf{W}} \ell(W, \mathbf{x})$
 - Faire un pas de SGD :

$$\mathbf{W} \leftarrow \mathbf{W} - \gamma \mathbf{g}$$

Comment optimiser le réseau ?

$$L(\mathbf{W}) = \sum_{\mathbf{x} \in \mathcal{E}} \ell(\mathbf{x}, \mathbf{W})$$

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-
- époque = désigne un passage complet du jeu de données d'entraînement par l'algorithme.
 - batch = morceau du jeu de données
 - Pour cette raison, input d'un réseau de la forme $[b, c, M, N]$
 - Comment est calculé le gradient ?

Un paramètre supplémentaire : le moment (momentum)

- Pour chaque époque :
 - Pour chaque batch \mathcal{B} de l'ensemble de données d'entraînement, pris dans un ordre aléatoire
 - Calculer $\ell(W, \mathbf{x})$ pour \mathbf{x} dans le batch
 - Calculer $\mathbf{g} = \beta \mathbf{g} + (1 - \beta) \sum_{\mathbf{x} \in \mathcal{B}} \nabla_{\mathbf{W}} \ell(W, \mathbf{x})$
 - Faire un pas de SGD :

$$\mathbf{W} \leftarrow \mathbf{W} - \gamma \mathbf{g}$$

→ C'est une façon d'accélérer la convergence

Questions?

Sources, images courtesy and acknowledgment

Charles Deledalle

V. Lepetit

L. Masuch